Mat. Res. Soc. Symp. Proc. Vol. 692 © 2002 Materials Research Society K5.6

Simulations of Realizable Photonic Bandgap Structures with High Refractive Contrast

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ABSTRACT

The transfer matrix method (TMM) software (Translight, A. Reynolds [1]) was used to evaluate the photonic band gap (PBG) properties of the periodic arrangement of high permittivity ferroelectric composite (40 wt% $Ba_{0.45}Sr_{0.55}TiO_3$ /60 wt% MgO composite, $\varepsilon_R = 80$, $\tan\delta = 0.0041$ at 10 GHz) in air (or Styrofoam, $\varepsilon_R \sim 1$) matrix compared to a lower permittivity material (Al_2O_3, $\varepsilon_R = 11.54$, $\tan\delta = 0.00003$ at 10 GHz) in air. The periodic structures investigated included a one-dimensional (1D) stack and a three-dimensional (3D) face centered cubic (FCC) opal structure. The transmission spectrum was calculated for the normalized frequency for all incident angles for each structure. The results show that the bandgaps frequency increased and the bandgap width increased with increased permittivity. The effects of orientation of defects in the opal crystal were investigated. It was found by introducing defects propagation bands were introduced. It was concluded that a full PBG is possible with the high permittivity material.

INTRODUCTION

Photonic crystals (PCs) are periodic dielectric structures that exhibit frequency ranges over which an electromagnetic waves cannot propagate (called a bandgap). They are composites that are artificially engineered to have a periodic variation in the dielectric constant with a period that is on the order of the electromagnetic (EM) wavelength. When the phases have a strong refractive contrast (>3), a bandgap is created in the frequency spectrum due to the Bragg-like reflection at the interface between the two phases. PCs have many applications in optical devices including waveguides, lasers, light-emitting diodes, couplers, and filters [2]. They have also been used in microwave devices for high efficiency antenna substrates and reflectors [3] as well as waveguides, filters and delay lines. Typically, silicon has been the material of choice. It has both a high dielectric contrast ($\varepsilon_R = 12.0{:}1$) and is compatible with fabrication methods in microelectronic and optical components. However, in this paper we propose using an even higher dielectric material, 40 wt% $Ba_{0.45}Sr_{0.55}TiO_3$ / 60 wt% MgO composite ($\varepsilon_R = 80$, $\tan\delta = 0.0041$ at 10 GHz [4]). Because $Ba_{0.45}Sr_{0.55}TiO_3$ is also a ferroelectric material whose permittivity changes under an applied electric field, it is also possible to electronically tune the position and width of the bandgap.

In order to prepare a PC, the material must be periodic within less than 5% deviation. Therefore in order to obtain the correct length-scale for the desired bandgap, a model of the structure and simulation of the EM propagation must first be made. Many numerical approaches are described in the literature [5] including the plane wave method, transfer matrix method (TMM) and finite difference time domain (FDTD) method. The plane wave method was developed by expanding the EM fields as a sum of plane waves and recasting Maxwell's equations in the form of an eigenvalue problem to find the allowed eigen-frequencies. This can be represented by the equation (1):

$$-\nabla^2 E + \nabla(\nabla \bullet E) = \omega^2 \varepsilon(r) E(r)$$

where E is the electric field, ω is the frequency, ε is the dielectric function and r is the coordinate. The disadvantages of this method are that it is inefficient in calculating complicated defects and requires significant computer time [5]. It is used to calculate the band diagrams, the field distributions and energy flows [5]. The FDTD method is the most widely used code [5] and requires less computer time [6]. However, it is inaccurate for modeling curvature and small objects. In the FDTD method, the wave propagating through the structure is found by integrating the discrete form of Maxwell's equations in the time domain. It is most often used for calculating reflection-transmission spectrums, band diagrams, field distributions, energy flows, and for coupling problems [5]. In TMM the wave-field is represented as points of real space lattice that relate the fields of one layer of the lattice to the next. The form of Maxwell's equation that this system takes on in three dimensions would be the following six equations (2-7) [7]:

$$\frac{E_y(\mathrm{r}+\mathrm{a}) - E_y(\mathrm{r})}{ia} - \frac{E_x(\mathrm{r}+\mathrm{b}) - E_x(\mathrm{r})}{ib} = \omega\mu(\mathrm{r})\mu_o H_z$$

$$\frac{E_z(\mathrm{r}+\mathrm{b}) - E_z(\mathrm{r})}{ib} - \frac{E_y(\mathrm{r}+\mathrm{c}) - E_y(\mathrm{r})}{ic} = \omega\mu(\mathrm{r})\mu_o H_x$$

$$\frac{E_x(\mathrm{r}+\mathrm{c}) - E_x(\mathrm{r})}{ic} - \frac{E_z(\mathrm{r}+\mathrm{a}) - E_z(\mathrm{r})}{ia} = \omega\mu(\mathrm{r})\mu_o H_y$$

$$\frac{H_z(\mathrm{r}-\mathrm{b}) - H_z(\mathrm{r})}{ib} + \frac{H_y(\mathrm{r}-\mathrm{c}) - H_y(\mathrm{r})}{ic} = -\omega\varepsilon(\mathrm{r})\varepsilon_o E_x$$

$$\frac{H_x(\mathrm{r}-\mathrm{c}) - H_x(\mathrm{r})}{ic} + \frac{H_z(\mathrm{r}-\mathrm{a}) - H_z(\mathrm{r})}{ia} = -\omega\varepsilon(\mathrm{r})\varepsilon_o E_y$$

$$\frac{H_y(\mathrm{r}-\mathrm{a}) - H_y(\mathrm{r})}{ia} + \frac{H_x(\mathrm{r}-\mathrm{b}) - H_x(\mathrm{r})}{ib} = -\omega\varepsilon(\mathrm{r})\varepsilon_o E_z$$

where μ is the permeability, a,b,c are the displacement through a distance along the x, y, z axis, respectively. TMM is most often used to calculate the reflection-transmission spectrums, and the field distributions [5].

The objective of this research was to model the PC of a 1D Bragg stack and a 3D opal using TMM comparing a high permittivity material (40 wt% $Ba_{0.45}Sr_{0.55}TiO_3$ / 60 wt% MgO composite, $\varepsilon_R = 80$, $\tan\delta = 0.0041$ at 10 GHz) in air (or Styrofoam, $\varepsilon_R \sim 1$) matrix compared to a lower permittivity material (Al_2O_3, $\varepsilon_R = 11.54$, $\tan\delta = 0.00003$ at 10 GHz) in air and to evaluate the effects of line defects and orientation on the propagation.

MODELING

A transfer matrix method software package called Translight [1] was used to model the PBG structures. The structures investigated were a 1D Chigrin's Stack [8] and 3D <111> opal [9]. The permittivities investigated were ε_R=80, 11.54 and $\tan\delta$ = 0.0041, 0.00003, respectively, corresponding to the materials of ferroelectric 40 wt% $Ba_{0.45}Sr_{0.55}TiO_3$ /60 wt% MgO composite

and Al_2O_3, respectively. For both structures a lattice constant of 0.003 m was used to calculate the transmission through the structure as a function of incident angle from 0 to 90 degrees and normalized frequency, fa/c, from 0.01 to 1.0, where f is the frequency, a is the lattice constant and c is the speed of light. The results were displayed on a contour plot with transmission in gray scale. Positive incident angles correspond to TM polarized waves while the negative values correspond to TE polarized waves unless otherwise reported.

The Chigrin's stack consisted of alternating layers of air (0.5 – 0.25 thick) and dielectric (0.75 thick) see. Figure 1a. The stacks were placed in x axis orientation relative to the incident beam. The opal structure PBG was investigated for filling factors 0.25, 0.5 and 0.74. For these simulations there were twelve stacks of a group of three unit cells with twenty-seven atom spheres each (cf. Figure 1b). Because the opal cell was symmetric along x, y, and z only the affect of orientation with a defect in the structure was considered. A defect was placed on each of the unit cells at the half-way point by removing the row of atoms along the y axis.

Figure 1: PBG Structures a. Chigrin's Stack, b. Opal Unit Cell.

RESULTS AND DISCUSSION

The effect of permittivity on the Chigrin's Stack are compared for ε=80 and ε=11.54 in Figures 2a and 2b, respectively. As shown in the figures, as the permittivity increases the number of bandgaps increases and the bandgap width increases.

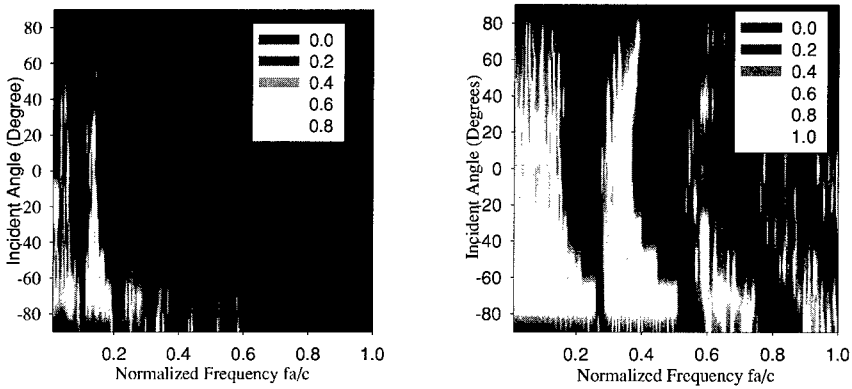

Figure 2. Chigrin's Stack with x Axis Orientation and 0.5 stack size and a. ε=80 and b. ε=11.54.

Similarly, the effect of increasing the stack size in a Chigrin's stack from 0.5 (cf. Figure 2a) to 0.75 (cf. Figure 3) shows an increase in the number of bandsgaps as well as an increase in the bandgap width.

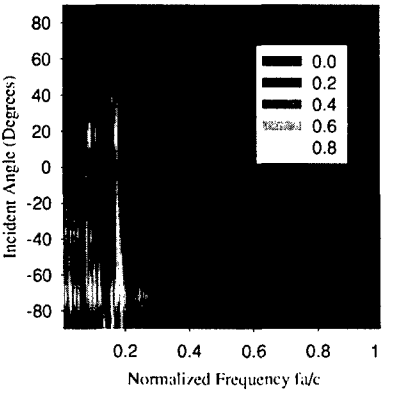

Figure 3. Chigrin's Stack Results with a Block Size of 0.75 and ε=80 and x Axis Orientation.

A comparison of the permittivity on the PBG of the opal structure with a defect is shown in Figures 4a and 4b. Without the defect the opal structure does not have the extra propagation bands at higher frequency (cf., enclosed circle of Figure 4a). These propagation bands can be used to trap and guide the electromagnetic radiation.

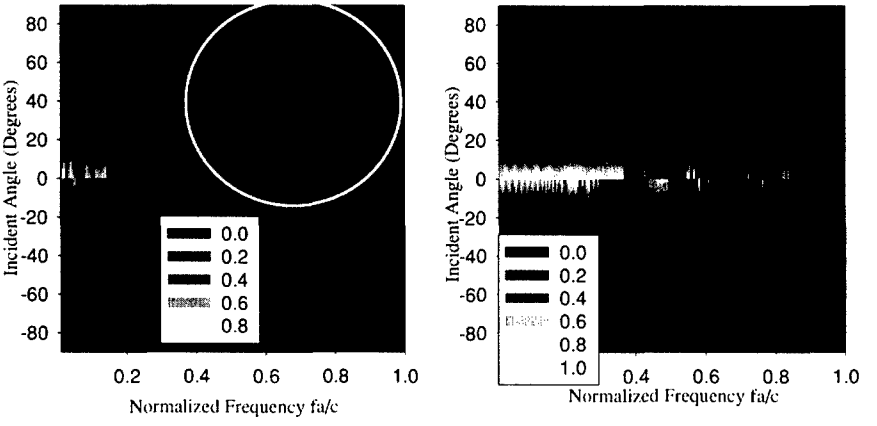

Figure 4. Opal structure PBG with 0.74 filling fractions a. ε=80 and b. ε=11.54.

The effect of increasing the filling fraction in the opal structure is shown in Figure 5. As the filling fraction decreases the number of bandgaps increases and the bandgap width increases.

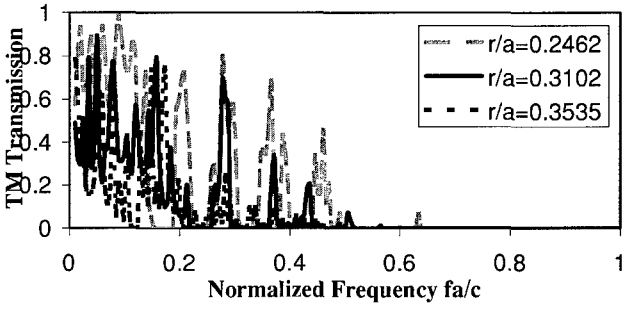

Figure 5. The effect of filling fraction on the PBG of the opal with ε=80 and no defect.

SUMMARY

A TMM software package was used to model the PBG structures of a Chigrin's Stack and <111> opal. The permittivities investigated were ε_R=80 and 11.54 and tanδ = 0.0041 and 0.00003, respectively, corresponding to the materials of ferroelectric 40 wt% $Ba_{0.45}Sr_{0.55}TiO_3$ /60 wt% MgO composite and Al_2O_3, respectively. Calculations of the transmission through the structure as a function of incident angle and normalized frequency were performed. It was found that the bandgaps increased and the bandgap width increased with increased permittivity. The effects of orientation of defects in the crystal were investigated. It was found by introducing defects propagation bands were introduced. It was concluded that a full PBG is possible with the high permittivity material.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the helpful technical discussions of Professor Azriel Genack, Bing Hue from Queens College, CUNY; Professor Dennis Prather of the University of Delaware and Dr. Mihail Sigalas of Agilent Laboratory.

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